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Supporting information for article:

Nitrosative stress sensing in *Porphyromonas gingivalis*: structure and heme binding by the transcriptional regulator HcpR

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Table S1 Primers used in this study

Primers for Cloning	
pET21-*hcpR*-Forward	CTTCCAGGGATCCCCAGAATTCGATCTTC
pET21-*hcpR*-Reverse	GCGCACTCGAGTTACTCCAGCCTCGACA
pFC20K-*hcpR*-Forward	TTGTGTTTAAACCTCCAGCCTCGACAA
pFC20K-*hcpR*-Reverse	GCCGGCGATCGCCATGGATCCCGAAT

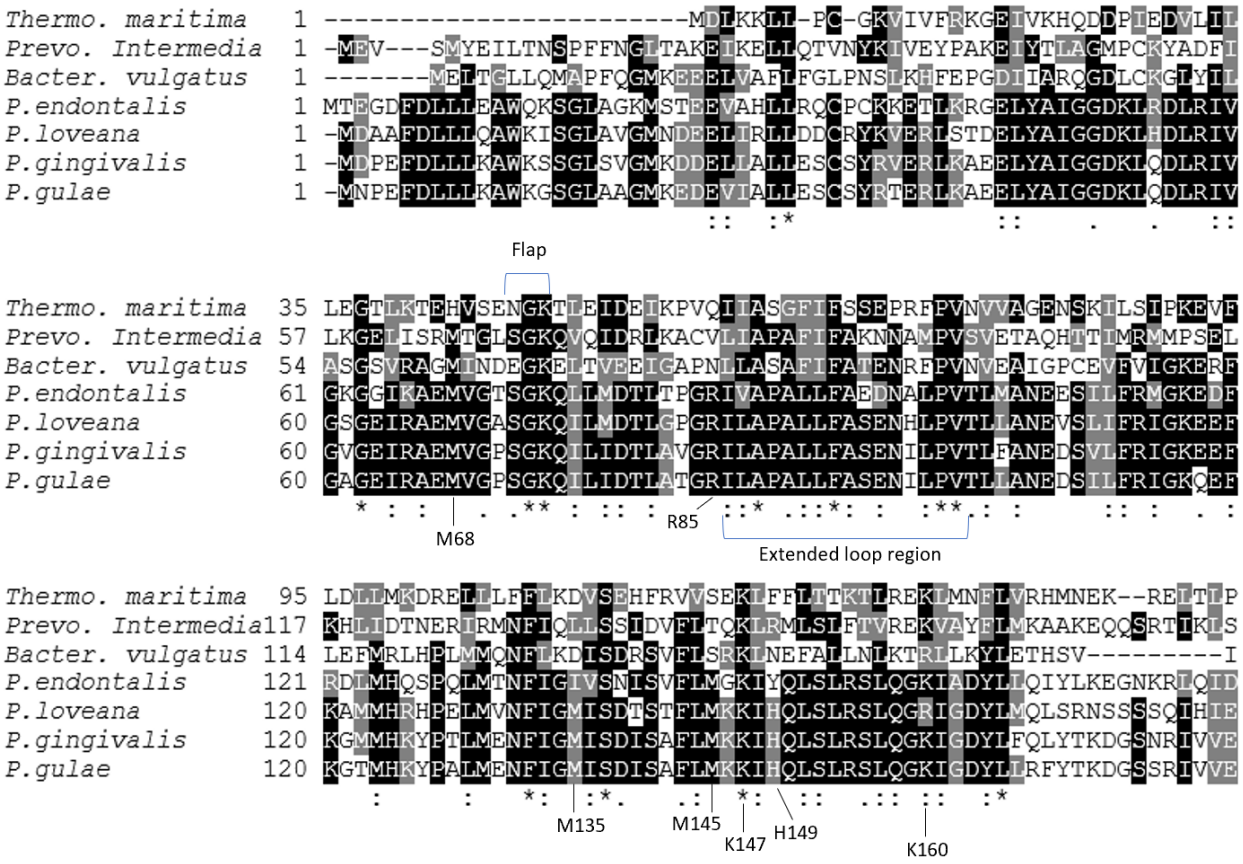


Figure S1 Sequence alignment of the HcpR sub-family. *P. gingivalis* HcpR aligned with putative HcpRs of related species. Pocket residues shown in Fig. 2B are labeled as well as other structural features.

Figure S2 Full sequence alignment of HcpR-DNR and HcpR-CooA. A. Sequence alignment of HcpR and DNR. The residue implicated in heme axial coordination in DNR is boxed in green (His187). B. Sequence of alignment of HcpR and CooA. The residues implicated in heme axial coordination in CooA are boxed in red (Pro3 and His77).

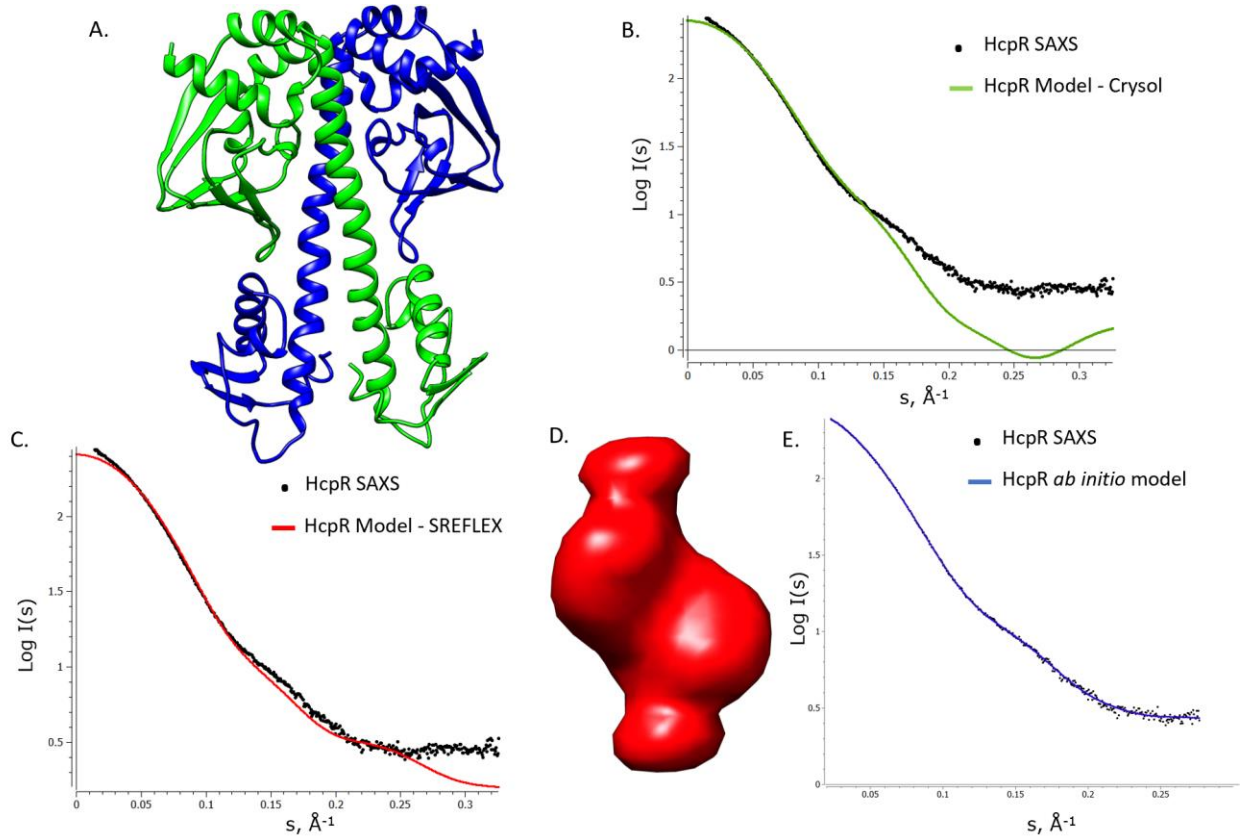


Figure S3 Chimeric model of full length HcpR and fitting to SAXS scattering data. A. The full-length chimeric model of HcpR. The DNA binding domain of DNR (PDB id: 3dkw) was used as a template to model the HcpR DNA binding domain. This was combined with the crystal structure of the HcpR sensing domain to create the full-length chimeric model. B. The theoretical scattering curve of the full-length HcpR model was fitted to the HcpR SAXS scattering data. The curves have a χ^2 value of 38.09. C. The full-length model was refined using SREFLEX. The theoretical scattering curve of the best model fit the HcpR SAXS scattering data with a χ^2 of 14.75. D. SAXS *ab initio* envelope of full-length HcpR created via DAMMIN. E. Theoretical scattering curve of the *ab initio* DAMMIN model fitted to the SAXS scattering data. The curves have a χ^2 value of 0.522. The *ab initio* model has an NSD of 3.1 with the chimeric full-length model.

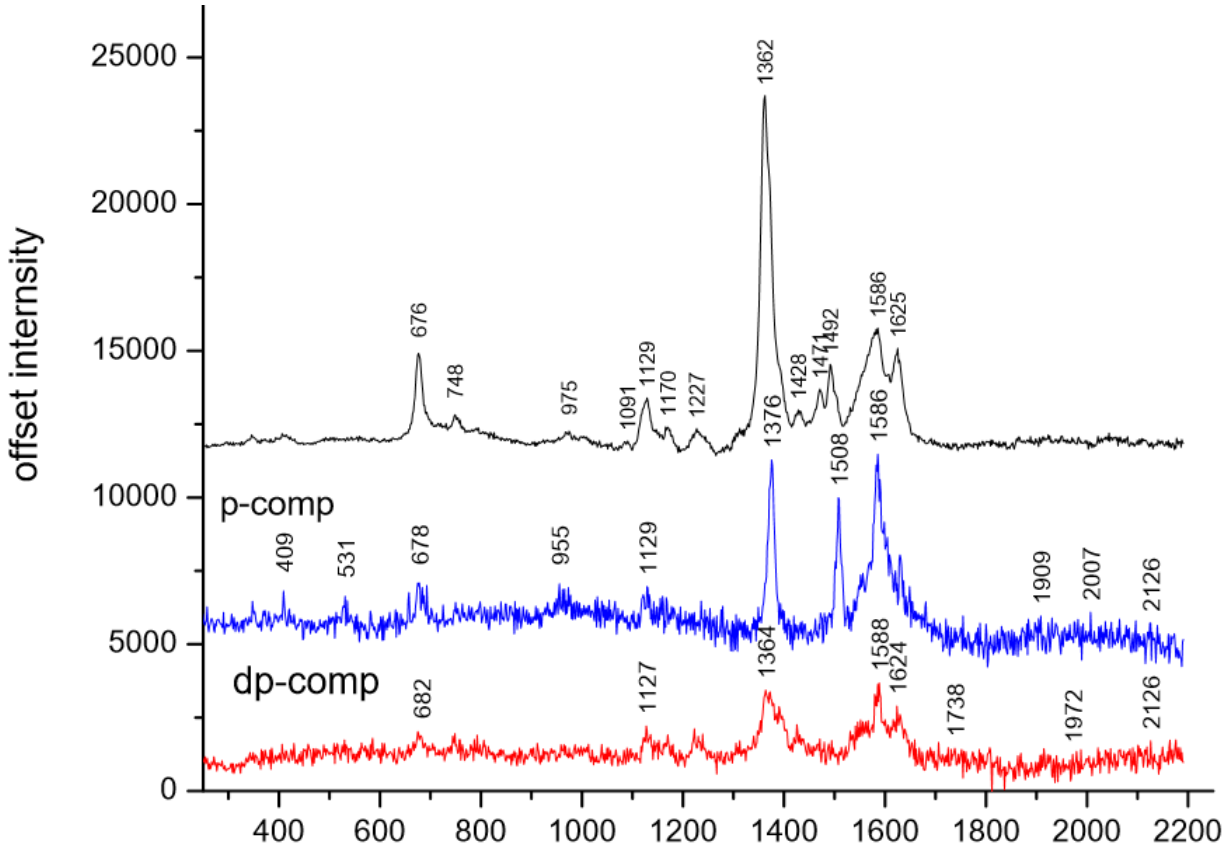
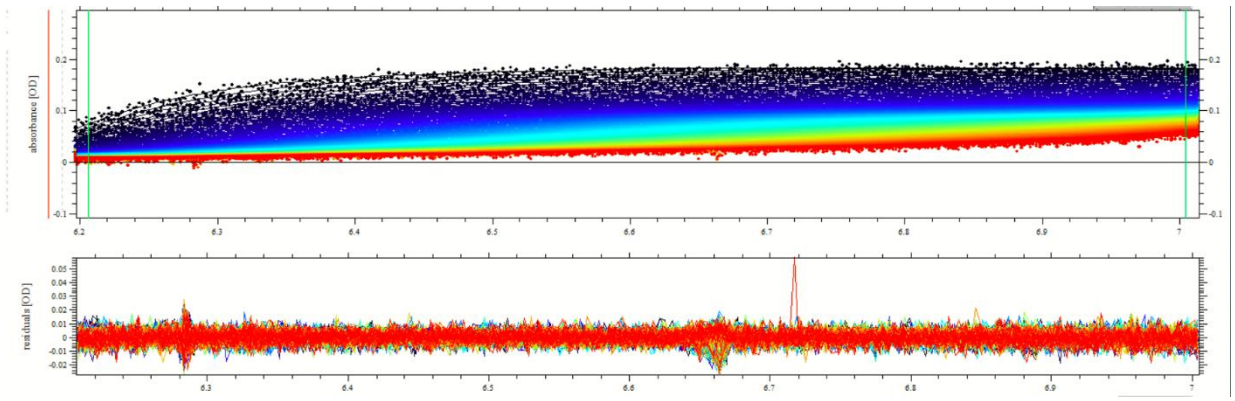


Figure S4 Polarizing and Depolarizing components. Polarizing (blue) and depolarizing (red) components of the resonance Raman spectrum (black) of the reduced heme bound form of HcpR.

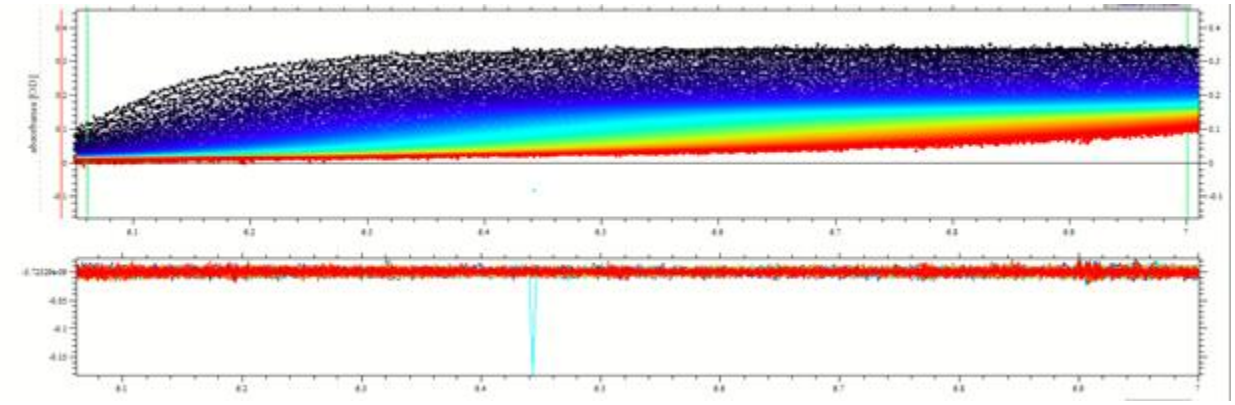
CELL 1



CELL 1

sw = 3.559 S, sw(20,w) = 3.631 S
(c = 0.0751, 40.147% of total)
with best-fit friction ratio = 1.287: Mw = 52090 Da
(based on vbar = 0.747, vbar20 = 0.747, hydration = 0.300, buffer
density = 1.00500, rel. viscosity = 1.0000)
minimum Mw (for compact sphere) = 35659 Da
Stokes Radius (20C) = 3.21 nm, a/b(oblate)=3.72, a/b(prolate)=3.53

CELL 2

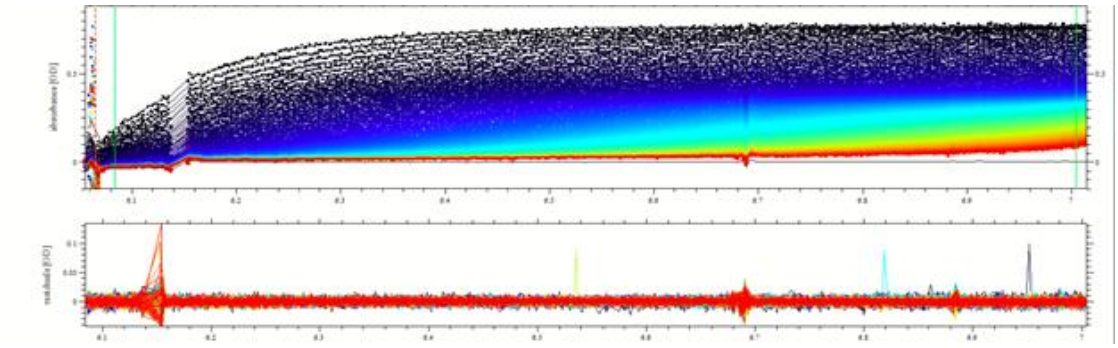


CELL 2

sw = 3.606 S, sw(20,w) = 3.680 S
(c = 0.1441, 41.790% of total)
with best-fit friction ratio = 1.332: Mw = 55848 Da
(based on vbar = 0.747, vbar20 = 0.747, hydration = 0.300, buffer
density = 1.00500, rel. viscosity = 1.0000)
minimum Mw (for compact sphere) = 36327 Da
Stokes Radius (20C) = 3.39 nm, a/b(oblate)=4.37, a/b(prolate)=4.11

Figure S5 Raw data of the sedimentation velocity experiments. Cell 1. 0.1mg/mL sample; Cell2. 0.2 mg/mL sample.

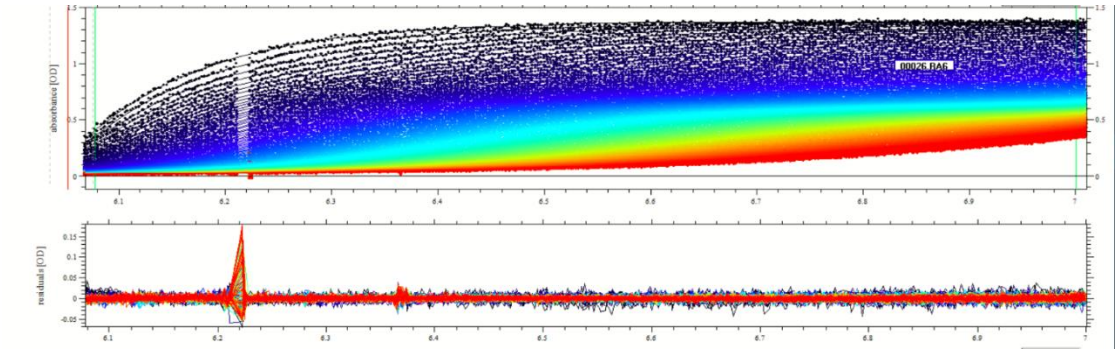
CELL 5



CELL 5

sw = 3.478 S, sw(20,w) = 3.548 S
(c = 0.5999, 42.426% of total)
with best-fit friction ratio = 1.359: Mw = 54513 Da
(based on vbar = 0.747, vbar20 = 0.747, hydration = 0.300, buffer
density = 1.00500, rel. viscosity = 1.0000)
minimum Mw (for compact sphere) = 34399 Da
Stokes Radius (20C) = 3.44 nm, a/b(oblate)=4.77, a/b(prolate)=4.46

CELL 6



CELL 6

sw = 3.552 S, sw(20,w) = 3.624 S
(c = 0.3521, 44.555% of total)
with best-fit friction ratio = 1.268: Mw = 50690 Da
(based on vbar = 0.747, vbar20 = 0.747, hydration = 0.300, buffer
density = 1.00500, rel. viscosity = 1.0000)
minimum Mw (for compact sphere) = 35507 Da
Stokes Radius (20C) = 3.13 nm, a/b(oblate)=3.44, a/b(prolate)=3.28

Figure S6 Raw data of the sedimentation velocity experiments. Cell 5. 0.5mg/mL sample; Cell6 . 1.0 mg/mL sample.